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Alan E. Gelfand

ABSTRACT

For the problem of individual prediction in linear regression models, that is, estimation of a linear combination of regression coefficients, mean square error behavior of a general class of adaptive predictors is examined.

1. INTRODUCTION

Suppose the usual linear regression model with fixed regressors, $Y = X\beta + \varepsilon$, $Y_{n\times 1}$, $X_{n\times p}$ full rank, $\beta_{p\times 1}$ and $\varepsilon_{n\times 1} \sim (0,\sigma^2 I)$. Let $\hat{\beta}_{LS} = (X^T X)^{-1} X^T Y$ denote the ordinary least squares estimator of β. At a new vector of predictor values, $\underline{X}_0$, we seek to estimate $\underline{X}_0^T\beta$. Using mean square error as a criterion, results of Cohen (1965) show that if ε is normally distributed, $\alpha\underline{X}_0^T\hat{\beta}_{LS}$ is an admissible estimator of $\underline{X}_0^T\beta$ for $0 \leq \alpha \leq 1$, e.g., the UMVU predictor is admissible. In fact, a predictor of the form $\ell^T Y$ is admissible for $\underline{X}_0^T\beta$ iff $(2\ell - X(X^T X)^{-1}\underline{X}_0)^T(2\ell - X(X^T X)^{-1}\underline{X}_0 \leq \underline{X}_0^T(X^T X)^{-1}\underline{X}_0$.

In the sequel, we study the MSE under normality of predictors of the form $\underline{X}_0^T\hat{\beta}_C$ where

$$\hat{\beta}_C = C\hat{\beta}_{LS} + (I - C)\beta^* \qquad (1)$$

C a matrix usually data dependent and β^* a specified vector. Such $\hat{\beta}_C$ include most alternatives to $\hat{\beta}_{LS}$ discussed in the literature. Earlier work in this direction appears in Baranchik (1964) and Radhakrishnan (1970).

2. NOTATION AND MOTIVATION

To simplify matters, we convert to canonical form. Let $\hat{\alpha} = P\hat{\beta}_{LS}$, P orthogonal such that $P(X^TX)^{-1}P^T = D^{-1}$, D diagonal with diagonal elements d_i. Define $\alpha = P\beta$, $\ell = P\underset{\sim}{X}_0$ and for convenience set $\beta^* = 0$. For the moment assume σ^2 known. Our problem now is to estimate $\theta = \ell^T\alpha$ given $\hat{\alpha} \sim N(\alpha, \sigma^2 D^{-1})$ wishing to do well near $\theta = 0$. Let $U = \ell^T\hat{\alpha}$, $Z = \hat{\alpha}^T D\hat{\alpha}$, $q = \ell^T D^{-1}\ell$, $V = Z - U^2/q$, $\lambda = \alpha^T D\alpha$ and $\zeta = \lambda - \theta^2/q$. Then, U, V are independent, $U \sim N(\theta, \sigma^2 q)$, $V \sim \sigma^2\chi^2_{p-1}(\zeta/\sigma^2)$.

Consider a general adaptive predictor $\delta(\hat{\alpha})$ of the form

$$\delta(\hat{\alpha}) = \Sigma h_i(\hat{\alpha})\ell_i\hat{\alpha}_i. \tag{2}$$

Most predictors of θ discussed in the literature are special cases of (2). Apart from the LS predictor, U, we have:

i) A class of predictors given in Thompson (1968)

$$T_m = \frac{U^2}{U^2+m\sigma^2 q}U, \text{ m a known constant, i.e., } h_i(\hat{\alpha}) = \frac{(\hat{\alpha}^T\ell)^2}{(\hat{\alpha}^T\ell)^2+m\sigma^2 q}.$$

ii) A class of predictors given in Mehta and Srivastava (1971)

$$MS_{b_1,b_2} = (1-b_1 e^{-b_2U^2/\sigma^2 q})U,\ 0 < b_1 < 1,\ b_2 > 0,\ b_1, b_2 \text{ known},$$

$$\text{i.e., } h_i(\hat{\alpha}) = 1 - b_1 \exp(-b_2(\hat{\alpha}^T\ell)^2/\sigma^2 q).$$

iii) A predictor arising from the James-Stein estimator adapted for unequal variances (Sclove 1968)

$$JS_c = (1 - \frac{c\sigma^2}{Z})U, \text{ c known usually taken equal to } p - 2.$$

A positive part adjustment should be applied so that $h_i(\hat{\alpha}) = [1 - c\sigma^2(\hat{\alpha}^T D\hat{\alpha})^{-1}]^+$.

iv) Predictors arising from (simple) ridge estimators

$$R_{k_t} = \Sigma \ell_i \frac{d_i}{d_i + k_t} \hat{\alpha}_i$$

where k_t is based on the data, i.e., $h_i(\hat{\alpha}) = d_i/(d_i+k_t(\hat{\alpha}))$. k's discussed include:

$k_1(\hat{\alpha}) = \sigma^2 p(\hat{\alpha}^T\hat{\alpha})^{-1}$ (Hoerl, Kennard, and Baldwin 1975),

$k_2(\hat{\alpha}) = \sigma^2 p Z^{-1}$ (Lawless and Wang 1976),

$k_3(\hat{\alpha})$, the solution to $\Sigma\hat{\alpha}_i^2 d_i^2 (d_i + k_3)^{-2} = \Sigma\hat{\alpha}_i^2 - \sigma^2 \Sigma d_i^{-1}$

(McDonald and Galarneau 1975),

$k_4(\hat{\alpha})$, the solution to $\Sigma\hat{\alpha}_i^2 d_i (d_i + k_4)^{-1} = \sigma^2 p$

(the RIDGM estimator of Dempster, Schatzoff and Wermuth 1977).

A subclass of (2) which includes (i), (ii), (iii), and R_{k_2} has the form

$$\delta(\hat{\alpha}) = \Sigma h_i(U,Z)\ell_i\hat{\alpha}_i \ . \tag{3}$$

A further subclass which still includes (i), (ii), and (iii) is

$$\delta(\hat{\alpha}) = h(U,Z) \cdot U. \tag{4}$$

When D = I, all of the aforementioned estimators belong to (4).

Taking another point of view (see e.g. Thompson (1968)), if h_i in (3) is constant, the optimal h_i to minimize the MSE are easily obtained:

$$h_i^* = \frac{\theta}{\sigma^2 + \lambda} \frac{\alpha_i}{\ell_i} \ . \tag{5}$$

An estimator of h_i^* would be of the form $c_i(\hat{\alpha},\sigma^2)$ leading to a predictor belonging to (2). If (5) was estimated by $c(U,Z,\sigma^2) \cdot \hat{\alpha}_i/\ell_i$ the class (4) results.

Suppose we take a Bayesian approach using a prior which centers θ at 0, where we want to do well. More precisely, let Q be an orthogonal matrix such that $QD^{\frac{1}{2}}\alpha = \binom{\theta/\sqrt{q}}{\eta}$ where η is $(p - 1) \times 1$ and $\eta^T\eta = \phi$. If we take as our prior

$$\binom{\theta/\sqrt{q}}{\eta} \sim N\left(0,\begin{pmatrix}\gamma & 0\\ 0 & \rho\gamma I_{p-1}\end{pmatrix}\right),\ \rho \text{ known},$$

then under squared error loss, the Bayes estimate of θ is $(\gamma + \sigma^2)^{-1} \cdot \gamma U$. Since (U,Z) is sufficient under the marginal distribution of $\omega = QD^{\frac{1}{2}}\hat{\alpha}$ an "empirical Bayes" estimator of θ takes the form in (4).

3. EXAMINATION OF THE MSE

We can calculate the MSE for the general predictor in (2) in terms of the h_i, assuming σ^2 known.[1]

Theorem 1. If $E\left|\frac{\partial h_i}{\partial U} \cdot \hat{\alpha}_i\right| < \infty$, $i = 1,2,\ldots,p$,

$$\begin{aligned}\mathrm{MSE}(\delta) &= \sigma^2 q + E(\delta - U)^2 - 2\sigma^2 E\Sigma\ell_i^2(1 - h_i)\\ &\quad + 2\sigma^2 qE\Sigma\ell_i\hat{\alpha}_i \frac{\partial h_i}{\partial U}\ .\end{aligned} \tag{6}$$

Proof. By direct calculation

$$\mathrm{MSE}(\delta) = \sigma^2 q + E(\delta - U)^2 - 2E\{r(\hat{\alpha})(U - \theta)\} \tag{7}$$

where $r(\hat{\alpha}) = \Sigma(1 - h_i)\ell_i\hat{\alpha}_i$. Stein's identity (Stein 1981, p. 1148) converts the right-most term of (7) to $\sigma^2 qE(\frac{\partial r(\hat{\alpha})}{\partial U})$. Simplification yields (6).

$\frac{\partial h_i}{\partial U}$ *would be calculated using the transformation* $\hat{\alpha} = D^{-\frac{1}{2}}Q^T\omega$ of the previous section. In the case of (3), it can be calculated directly writing h_i as a function of U and V. For predictors of the form (4), MSE(δ) depends only on θ and ϕ and is given as Corollary 1.

Corollary 1. For the predictors in (4), if $E\left|U \frac{\partial h}{\partial U}\right| < \infty$

$$\mathrm{MSE}(\delta) = \sigma^2 q + E(1 - h)^2U^2 + 2\sigma^2 qEU \frac{\partial h}{\partial U} - 2\sigma^2 qE(1 - h). \tag{8}$$

Under (4) choices of h in the literature are such that h is symmetric in U about 0 and restricted to $[0,1]$. Using essentially the argument of Efron and Morris (1976, p. 14) positive part restriction of h uniformly reduces risk. Restriction of $h \leq 1$ is less clear. Taking $h > 0$ the predictor $h^* \cdot U$ where $h^* = \min(h,1)$ does not necessarily dominate $h \cdot U$. For example, let $h(U,V) = \begin{cases} 1 + c, & a^2 < U^2 < b^2 \\ 1 & , \text{elsewhere} \end{cases}$. Then at each ϕ, for $|\theta|$ sufficiently large, MSE of $h(U,V)U$ is less than MSE of $h^*(U,V)$. Nonetheless, to improve in a neighborhood of a specified θ_0 requires convex combinations of U and θ_0. Theorem 2 details MSE properties of predictors in (4) relative to the MSE of U.

Theorem 2. For $\delta(\hat{\alpha})$ in (4) with $h \in [0,1]$, let h be symmetric in U about 0. Let $g = (1 - h)U$ with $\lim_{|U|\to\infty} \sup_{V} g = 0$ and assume $\frac{\partial g}{\partial U}$ exists for all U. Finally, assume that the Lebesgue measure of $A = \{(U,V) : h(U,V) < 1\}$ is greater than 0. Then,

(i) For each ϕ there is a neighborhood N_ϕ of $\theta = 0$ where $MSE(\delta;\theta,\phi) < \sigma^2 q$.

(ii) $MSE(\delta;\theta,\phi)$ is bounded and $\lim_{|\theta|\to\infty} MSE(\delta;\theta,\phi) = \sigma^2 q$.

(iii) $MSE(\delta;\theta,\phi)$ is symmetric in θ about 0 and $\left.\frac{\partial MSE(\delta;\theta,\phi)}{\partial\theta}\right|_{\theta=0} = 0$.

(iv) $g^2 - 2\frac{\partial g}{\partial U}$ changes sign at least once in $0 < U < \infty$. If $g^2 - 2\frac{\partial g}{\partial U}$ changes sign b times in $0 < U < \infty$, then for fixed ϕ, $MSE(\delta;\theta,\phi) - \sigma^2 q$ changes sign at most 2b times.

Proof. The proof of (i) is clear since $MSE(\delta;0,\phi) < \sigma^2 q$. For (ii),

$$MSE(\delta;\theta,\phi) = \sigma^2 q + Eg^2 - 2E(U - \theta)g. \tag{9}$$

Given ε, $\exists\, u_0$ such that for all V, $U > u_0 \Longrightarrow |g| < \varepsilon$ and $\exists\, \theta_0 > 0$ such that $|\theta| > \theta_0 \Longrightarrow P(|U| > u_0) > 1 - \varepsilon$. Then the second term and the third term (using the Cauchy-Schwarz Inequality) in (9) can be made arbitrarily small as $|\theta| \to \infty$. It is clear that the r.h.s. of (9) is bounded. (iii) is obvious. The first part of (iv) follows since U is admissible. The second part follows from the sign change theorem of Karlin (1957) by noting that $\mathrm{MSE}(\delta;\theta,\phi) - \sigma^2 q = E(g^2 - 2\frac{\partial g}{\partial U})$.

Remark 1. Predictors in (i), (ii), (iii) of Section 2 satisfy the conditions of Theorem 2.

Remark 2. Result (ii) is a simple case of the "tail minimaxity" notion of Berger (1976).

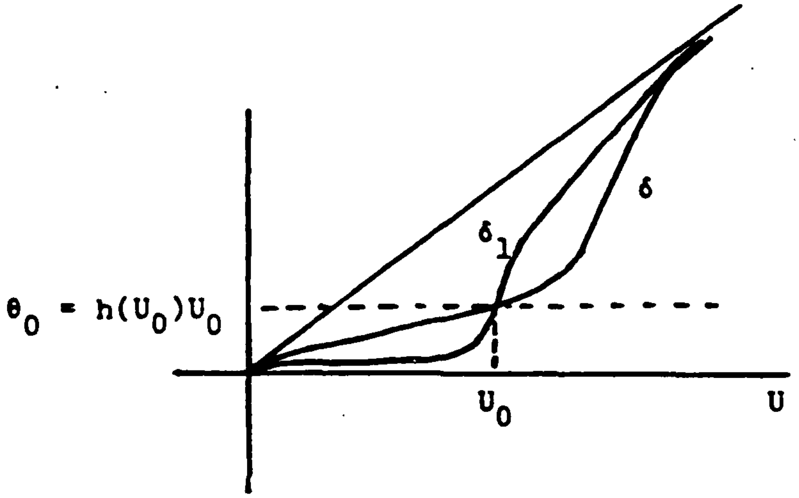
Remark 3. In (iii), $\inf_{\theta} \mathrm{MSE}(\delta;\theta,\phi)$ need not occur at $\theta = 0$. If, however, $h(U,V)$ is increasing in $|U|$ it must as may be shown by establishing the result for h, a step function in U. An induction argument proves this.

Remark 4. If $b = 1$ in (iv), then a graph of $\mathrm{MSE}(\delta;\theta,\phi)$ for $\theta \geq 0$ must start below $\sigma^2 q$ at $\theta = 0$, cross above $\sigma^2 q$ at some θ and then asymptotically return to $\sigma^2 q$ from above. Any predictor satisfying the conditions of Theorem 2 must necessarily perform worse for a set of θ's near 0 than for a set arbitrarily far away.

Remark 5. No immediate extension of Theorem 2 to $\delta(\hat{\alpha})$ as in (3) is available. For an arbitrary member of (3), MSE depends upon θ and η and, even if each h_i meets the "tail minimaxity" condition, need not approach $\sigma^2 q$ as $|\theta| \to \infty$ for fixed η.

Remark 6. Theorem 2 is readily extended to the comparison of any pair of predictors in (4).

We conclude with a comment on admissibility for the above predictors. Within the class of predictors based solely on U, i.e., $h(U)U$, those meeting the conditions of Theorem 2 will either be admissible or if not then improvement cannot be substantial. We employ ideas of Chow and Hwang (1984). Suppose $\delta_1(U)$ is to dominate $\delta_0 = h(U)U$ meeting the conditions of Theorem 2. We can write δ_1 as $h^*(U)U$, and assume $h^* \geq 0$. For δ_1 to dominate δ_0 requires, when $|U|$ is large, that generally h^* be closer to 1 than h and that, when $|U|$ is small, generally h^* be closer to 0 than h. A simplified picture of δ_0, δ_1 for $U > 0$ might look like



But, at $\theta = \theta_0$, it would be almost impossible for δ_1 to dominate. Thus, the simplest h* which realistically could dominate would have to have at least 3 sign changes for h - h* on $U > 0$. For such an h*, its form would be complicated, domination would be difficult to show, and improvement would be minimal.

This argument does not extend to the more general class (4). Though U and V are independent, conditioning on V in the above heuristic leads to θ_0 depending upon V. We, nonetheless, conjecture "approximate admissibility" for members of (4) meeting the conditions of Theorem 2.

FOOTNOTE

[1] When σ^2 is unknown, we customarily assume an estimator S^2 of σ^2 such that $\nu S^2 \sim \sigma^2\chi^2_\nu$ independent of $\hat{\alpha}$. In the foregoing predictors, σ^2 is replaced by cS^2. As Lawless (1981, pp. 463-464) notes, when $\nu \to \infty$ and even when ν is moderate, resulting MSE will differ little from that with σ^2 known.

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For the problem of individual prediction in linear regression models, that is, estimation of a linear combination of regression coefficients, mean square error behavior of a general class of adaptive predictors is examined.